

201-15210B1

I U C L I D

Data Set

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Existing Chemical : Substance ID: 44992-01-0
CAS No. : 44992-01-0
TSCA Name : Ethanaminium, *N,N,N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, chloride
Structural formula : CH2=CHCOOC2H4N(CH3)3.Cl
Molecular formula : C8H16NO2.Cl
Molecular weight : 193.6729

Producer related part
Company : Quat HPV Challenge Task Group
Creation date : 05.11.2003

Substance related part
Company : Quat HPV Challenge Task Group
Creation date : 05.11.2003

Number of pages : 35

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4

1. General Information

Id 44992-01-0

Date 05.11.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	: Organic.
Physical status	: Solid.
Purity	: > 99%.
Remark	: The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

05.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylacrylate, methyl chloride
05.11.2003

Choline chloride acrylate
05.11.2003

Dimethylaminoethyl acrylate methochloride
05.11.2003

[2-(acryloyloxy)ethyl]trimethylammonium chloride
05.11.2003

[(Acryloyloxy)ethyl]trimethylammonium chloride
05.11.2003

ADAMMC
05.11.2003

DMAEA MC
05.11.2003

1. General Information

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Date 05.11.2003

DMAEA MCQ
05.11.2003

1.3 IMPURITIES

Dimethylaminoethylacrylate (<0.1%).
05.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
05.11.2003

1.6.2 CLASSIFICATION

Not regulated.
05.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type	: Industrial.
Category	: Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	: Commercial product is manufactured and shipped as a solution in water (75–80%).

05.11.2003

1.7.1 DETAILED USE PATTERN

Used in closed system to manufacture polymers. Polymers are water-soluble and cationic and are either copolymers with acrylamide and other monomers or homopolymers.
05.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of methyl chloride with dimethylaminoethylacrylate.
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1. General Information

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1.8 REGULATORY MEASURES

None
05.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None.
05.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethylacrylate (ADAM) at less than 0.1%.
05.11.2003

1.8.3 WATER POLLUTION

Not applicable.
05.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable.
05.11.2003

1.8.5 AIR POLLUTION

Not applicable.
05.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).
05.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable.
05.11.2003

1.9.2 COMPONENTS

1. General Information

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Pure substance (in aqueous solution).
05.11.2003

1.10 SOURCE OF EXPOSURE

None.
05.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 44992-01-0

Date 05.11.2003

2.1 MELTING POINT

Value : =148.40°C.
Method : MPBPWIN v1.40.
Year : 2003.
GLP : No.
Test substance : ADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

07.11.2003

2.2 BOILING POINT

Value : =397.55°C
Method : MPBPWIN v1.40 (adapted Stein & Brown method).
Year : 2003.
GLP : No.
Test substance : ADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

07.11.2003

2.3 DENSITY

Type : Density.
Value : = 1.132 g/cm³ at 20°C (80% solution in water).
Method : Other: no data
Year : No data.
GLP : No data.
Test substance : ADAMMC (80% solution in water).
Reliability : (4) not assignable.
Only short information available (safety data sheet).

07.11.2003

2.3.1 GRANULOMETRY

Not applicable.
05.11.2003

2.4 VAPOUR PRESSURE

Value : =5.31 E-7 mm Hg at 25°C
Method : MPBPWIN v1.40 (modified Grain method).
Year : 2003.
GLP : No.
Test substance : ADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

2. Physico-Chemical Data

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2.5 PARTITION COEFFICIENT

Partition coefficient : Octanol-water.
log Pow : = -3.10
Method : KOWWIN v1.66.
Year : 2003
GLP : No.
Test substance : ADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water.
Value : 1 E6 mg/l at 25°C.
Method : WSKOW v1.40.
GLP : No.
Test substance : ADAMMC (pure substance)
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions. Additionally, no melting point equation was used.

07.11.2003

Solubility in : Water.
Value : Completely miscible.
Method : Other: no data.
GLP : No data.
Test substance : ADAMMC (pure substance)
Reliability : (4) not assignable.
Only short information available (safety data sheet).

07.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : Does not flash.
Method : Other: no data.
Year : No data.
GLP : No data.
Test substance : MADAM MC (80% solution in water).
Reliability : (4) not assignable
Only short information available (safety data sheet)

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2. Physico-Chemical Data

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2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	: 100 mPa.s
Method	: Other: no data.
GLP	: No data.
Test substance	: ADAMMC (80%).
Reliability	: (4) not assignable.

Only short information available (safety data sheet).

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2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Type : Air.
Method : AOPWIN v1.90.
Year : 2003.
GLP : No.
Result : The atmospheric degradation behavior was assessed using AOPWIN (v. 1.90). An overall OH rate constant of $25.5215 \text{E-12 cm}^3/\text{molecule} \cdot \text{sec}$ was obtained. The following half-lives can be predicted under the chosen conditions:
0.419 days (12h-day, $1.5 \text{E6 OH}/\text{cm}^3$); 5.029 hours.
Overall ozone rate constant = $0.175 \text{E-17 cm}^3/\text{molecule} \cdot \text{sec}$.
Half-life = 6.549 days (at $7 \text{E11 mol}/\text{cm}^3$)
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.
07.11.2003

3.1.2 STABILITY IN WATER

Type : Abiotic (hydrolysis).
Method : HYDROWIN v1.67
Year : 2003.
GLP : No.
Remark : The estimated hydrolysis half-life of this substance at:
pH 7 = 9.001 years;
pH 8 = 328.762 days
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.
07.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : Volatility.
Media : Water – air.
Method : HENRYWIN v3.10.
Year : 2003.
Remark : The value obtained for Henry's constant was calculated as:
Bond contribution method: $6.96 \text{E-15 atm} \cdot \text{m}^3/\text{mole}$ at 25°C (group contribution calculation incomplete). According to Thomas (1990), the substance may be considered as "not volatile from water".
Henry's LC (VP/WSol estimate using EPI values) = $1.353 \text{E-13 atm} \cdot \text{m}^3/\text{mole}$

3. Environmental Fate and Pathways

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Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

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Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	2.49 E-7	9.45	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44 E3	0

Persistence time = 421 hours.

Conclusion : Regardless of the media to which ADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of ADAMMC will be 54.6% in soil, 45.3% in water, <0.1% in sediment, and virtually nothing in air.

Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

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3.3.2 DISTRIBUTION

Media : Air – biota – sediment(s) – soil – water.
Method : Calculation according to Mackay, Level 1.
Year : No data.
Remark : The following parameters were employed in this calculation:
Vapor pressure: 1.8 E-5 Pa (20°C) (calculated);
Molecular weight: 207.7 g/mol;
water solubility: ca. 6000 g/l (20°C) (calculated);
logPow: -2.55 (25°C) (calculated).
Result : The following environmental distribution was predicted:
water: ca. 100%; other environmental compartments below 0.001%.
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

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3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : Aerobic.
Reference : Wehrhahn, D.
Inoculum : WWTP effluent.
Concentration : 60, 150 and 300 mg C/L.
Contact time : 27 days.
Degradation : = 85% after 27 days (average).

3. Environmental Fate and Pathways

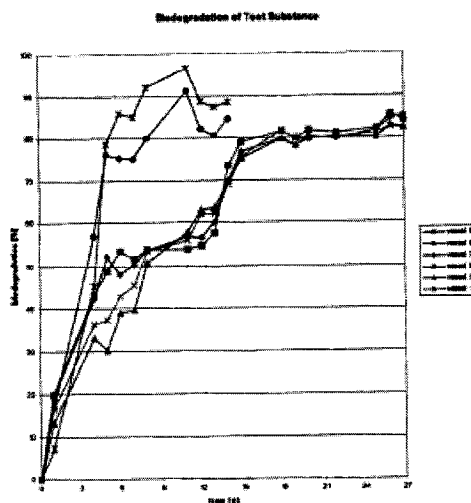
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Result : Inherently biodegradable.
Deg. product : Not measured.
Method : OECD Guidelines for the Testing of Chemicals, No. 302 B (1981) "Inherent Biodegradability: Zahn-Wellens Test".
Year : 1999
GLP : Yes
Test substance : Adame-Quat (80% solution in water)
Method : A mixture containing the test substance, mineral nutrients and a fairly large amount of activated sludge in aqueous medium were agitated and aerated at room temperature for 27 days. Blank controls containing activated sludge and nutrient but no test material were run in parallel as well as a positive control (4-Ethoxybenzoic acid). Biodegradation was monitored in both by DOC (Dissolved Organic Carbon) determination in filtered samples. The ratio of eliminated DOC (corrected using the control), measured at each time interval to the initial DOC was expressed as the percentage biodegradation during the time interval. The DOC was measured 3 times a week with a DOC analyzer.
The results of this study showed that the carbon content of the test substance is biodegraded as follows:

Nominal Concentration (mg/l)	Percentage Biodegradation
60	86.5 at 14 days
150	84.8 at 14 days
300	82.7 at 27 days

The rate of biodegradation for each test concentration is graphically represented below:



Test substance : ADAMMC (80% solution in water).
Conclusion : ADAMMC was characterized as ultimately biodegradable.
Reliability : (1) valid without restrictions.
Guideline study.

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(1)

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3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

- Type** : Static.
Species : *Brachydanio rerio* (Zebra Fish)(Fish, fresh water).
Reference : Calmels, R. (1994a).
Exposure period : 96 hours.
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, April 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : No.
Test substance : ADAME MECL
Test procedure : Groups of 10 fresh water Zebra Fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.
Results : The results are given in the following table:

Test Concentration (mg/L)	Mortality		
	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

- Test substance** : ADAMMC (80% solution in water).
Conclusion : Under the conditions of this test, the test substance is not harmful to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions.
 Guideline study.

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(2)

- Type** : Static.
Species : *Danio rerio* (Zebra Fish)(Fish, fresh water).
Reference : Wehrhan, D. (1999).
Exposure period : 96 hours.
Unit : mg/l
LC0 : 50
LC50 : 75
LC100 : 100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, April 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : Yes.

4. Ecotoxicity

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- Test substance** : Adame-Quat
- Test procedure** : The study was divided into a preliminary test over 48 hours and a main test over 96 hours. In the preliminary test the following nominal concentrations were used: 50, 100, 300, 700 and 1,000 mg/l. From 100 mg/l onward, mortalities were observed. Therefore, the main experiment was carried out with the following nominal concentrations: 50, 100, 150, 200, 250 and 300 mg/l. Nominal concentrations could not be verified because no specific analytical method was available. In the preliminary test, 5 fish were exposed to each concentration. In the main test, 10 fish were exposed to each concentration. The main test was carried out over 4 days. Mortalities and observable effects were recorded on a daily basis.

- Results** : The results are given in the following table:

Test Concentration (mg/L)	Mortalities			
	24 hours	48 hours	72 hours	96 hours
0	0	0	0	0
50	0	0	0	0
100	5	5	0	0
150	10	—	—	—
200	10	—	—	—
250	10	—	—	—
300	10	—	—	—

ADMMC was determined to have an LC50 at 96 hours of 75 mg/l, an LC100 of 100 mg/l and an LC0 of 50 mg/l.

Note: Slight deviations with respect to oxygen saturation occurred during the test (3% below required value).

- Test substance** : ADAMMC (80% solution in water).
- Conclusion** : Under the conditions of this test, the test substance has to be regarded as harmful (moderate concern) to *Danio rerio*.
- Reliability** : (1) valid without restrictions.

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(3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

- Type** : Static.
- Reference** : Calmels, R. (1994b).
- Species** : *Daphnia magna* (Crustacean, fresh water)
- Exposure period** : 48 hour(s)
- Unit** : mg/l
- EC0 (immobilization)** : > 100
- EC50 (immobilization)** : > 100 (Not observed).
- EC100 (immobilization)** : > 100 (Not observed).
- Analytical monitoring** : No.
- Method** : OECD Guidelines for the Testing of Chemicals, No. 202, Part 1, April 1984: "*Daphnia sp.*, Acute Immobilization Test".
- Year** : 1994
- GLP** : No.
- Test substance** : ADAME MECL
- Test procedure** : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test

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substance were used. Immobilized daphnia were counted after 24 and 48 hours.

Results

Concentration (mg/L)	No. of daphnia	Immobilization		
		No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMMC (80% solution in water)
Conclusion : Under the conditions of this test, the test substance is not harmful to *Daphnia magna* at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

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(4)

Type : Static.
Reference : Wehrhahn, D. (1999b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hour(s)
Unit : mg/l
EC0 (immobilization) : 40
EC50 (immobilization) : 120
EC100 (immobilization) : 320
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 202, Part 1, April 1984: "*Daphnia sp.*, Acute Immobilization Test".
Year : 1994
GLP : Yes.
Test substance : Adame-Quat
Test procedure : Groups of 25 new-born (age < 24 hours) *Daphnia magna* were exposed to nominal concentrations of 0, 5, 10, 20, 40, 80, 160 and 320 mg/l. Nominal concentrations could not be verified because no specific analytical method was available. Each group, including the control, was divided into 5 parallel groups of 5 organisms. The test was carried out over 2 days. On day one and day two, immobilized daphnia were counted and recorded.

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Results

Conc. (mg/L)	No. of daphnia	Immobilization			
		After 24 hours		After 48 hours	
		Number	%	Number	%
0	25	0	0	1	4
5	25	0	0	1	4
10	25	0	0	1	4
20	25	0	0	2	8
40	25	0	0	1	4
80	25	0	0	9	36
160	25	4	16	11	60
320	25	25	100	—	100

ADMMC was determined to have an EC50 at 48 hours of 120 mg/l, an EC0 of 50 mg/l and an EC100 of 320 mg/l.

According to the EPA trimmed Spearman-Kärber Method, the EC50s and their confidence limits are as follows

Point	Exposure Concentration	95% Confidence Limits	
		Lower	Upper
EC50 (24 hours)	202.52	182.95	224.19
EC50 (48 hours)	116.45	95.61	141.84

Test substance Conclusion

: ADAMMC (80% solution in water)
: Under the conditions of this test, the test substance has to be regarded as slightly toxic to *Daphnia magna*. The test substance is of low toxic concern with respect to the species.

Reliability

: (1) valid without restrictions
Guideline study.

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(5)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type

: Static.

Reference

: Licata-Messana, L. (1994).

Species

: *Scenedesmus subspicatus* (Algae, unicellular, fresh water).

Exposure period

: 72 hours.

Unit

: mg/l

EC_A50 (l)

: Between 1 and 10 mg/l.

EC_μ50 (l)

: Between 10 and 100 mg/l.

Analytical monitoring

: No.

Method

: OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth inhibition Test".

Year

: 1994

GLP

: No.

Test substance

: ADAME MECL

Test procedure

: Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test

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Results

substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

: The results are given in the following table:

GROWTH INHIBITION					
Concentration (mg/L)	Algal Concentration				% growth inhibition
	Start	24 hours	48 hours	72 hours	
0	10,000	188,340	2,248,344	13,850,004	0
1	10,000	380,004	1,923,336	12,283,332	11
10	10,000	230,004	806,676	2,933,340	79
100	10,000	180,000	306,672	300,012	98
GROWTH RATE INHIBITION					
Concentration (mg/L)	Growth rate		% growth rate inhibition		
0	0.0612		—		
1	0.0604		1		
10	0.0384		37		
100	0.0046		93		

The EC(I)50 at 72 hours was determined to be:

Growth inhibition: $1 < EC_{A50} < 10$

Growth rate inhibition: $10 < EC_{p50} < 100$.

Test substance

Conclusion

Reliability

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Type

Reference

Species

Exposure period

Unit

EC_{A50} (l)

EC_{p50} (l)

Analytical monitoring

Method

Year

GLP

Test substance

Test procedure

: ADAMMC (80% solution in water).

: Under the conditions of this test, the test substance has to be considered as toxic to algae.

: (1) valid without restrictions.

Comparable to guideline study.

(6)

: Static.

Wehrhahn, D. (1999c).

: *Scenedesmus subspicatus* (Algae, unicellular, fresh water).

: 96 hours.

: mg/l

: 1.1

: 0.8

: No.

: OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth inhibition Test".

: 1994

: Yes.

: Adame-Quat

: The test was carried out twice. In the first experiment the following concentrations were used: 0, 5, 10, 20, 40, 80, 160 and 320 mg/l. Nominal concentrations could not be verified since no specific analytical method was available. After 24 hours, no growth except in the control was observed, even in the lowest concentration. The test was stopped and carried out again with lower concentrations of the test substance and a control. each concentration and the control were prepared in quadruple. The nominal concentrations tested were 0.1, 0.2, 0.4, 0.8, 1.6, 3.2 and 6.4 mg/l. each

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Results

concentration and the controls were inoculated with approximately 10,000 algae per ml. The test was carried out over 96 hours. Once a day, the extinction of an aliquot of the test vessels was measured photometrically.

: The results are given in the following table:

Conc. (mg/L)	72 hours				96 hours			
	Area	Red (%)	Growth rate	Red (%)	Area	Red (%)	Growth rate	Red (%)
0	3.37	0	0.0541	0	8.27	0	0.0420	0
0.1	2.74	19	0.0496	8	7.03	15	0.0409	3
0.2	2.39	29	0.0590	-9	6.48	22	0.0480	-14
0.4	1.94	42	0.0573	-6	5.48	34	0.0488	-16
0.8	1.81	46	0.0604	-12	5.27	36	0.0510	-21
1.6	1.02	70	0.0513	5	3.12	62	0.0481	-15
3.2	0.53	84	0.0395	27	1.45	82	0.0409	3
6.4	0.19	94	0.0144	73	0.37	96	0.0237	44

The EC(I)50 at 72 hours was determined to be:

EC_A50 (growth)= 0.65

EC_P50 (growth rate) = 0.55

The EC(I)50 at 96 hours was determined to be:

EC_A50 (growth)= 1.1

EC_P50 (growth rate) = 0.8

Test substance

: ADAMMC (80% solution in water).

Conclusion

: Under the conditions of this test, the test substance has to be considered as toxic to algae.

Reliability

: (1) valid without restrictions.

Comparable to guideline study.

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(7)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type

: Static

Reference

Wehrhahn, D. (1999d)

Species

: *Pseudomonas putida* (Bacteria).

Exposure period

: 24 hours.

Unit

: mg/l

EC50

: = 586

Analytical monitoring

: No

Method

: DIN 38 412 Teil 8 (Bringmann-Kühn, 1977)

Year

: 1999

GLP

: Yes

Test substance

: Adame-Quat

Test procedure

: The test was carried out at 30°C with the following nominal concentrations: 0, 3, 6, 12, 24, 49, 98, 195, 391, 781, 1563, 3,125, 3,250 and 12,500, 50,000, 100,000, 200,000 and 400,000 mg/l. Nominal concentrations could not be verified since no specific analytical method was available. Each concentration and the control were prepared in duplicate. Each concentration was inoculated with 10 ml of a bacteria suspension with an extinction of 0.1 at $\lambda = 436$ nm. The bacteria were exposed to the test substance for 24 hours. Thereafter, an aliquot was taken from each test and

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control vessel, which was diluted and aliquots from the resulting solutions were pipetted into Petri dishes filled with King B medium. Bacteria were distributed by means of a Drigalski spatula. The Petri dishes were incubated for one day at 30°C. The growth of the bacterial colonies on the Petri dishes was evaluated macroscopically.

Results

: The results are given in the following table:

Concentration mg/l	Dilution factor	Growth at dilution of 10 ⁻²	
		Incubation A	Incubation B
control	control	+++	+++
400,000	1:2	–	–
200,000	1:4	–	–
100,000	1:8	–	–
50,000	1:16	–	–
25,000	1:32	–	–
12,500	1:64	–	–
6,250	1:128	–	–
3,125	1:256	–	–
1,563	1:512	++	++
781	1:1024	++	++
391	1:2048	+++	+++
195	1:4096	+++	+++
98	1:8192	+++	+++
49	1:16392	+++	+++
24	1:32784	+++	+++
12	1:65568	+++	+++
6	1:131136	+++	+++
3	1:262772	+++	+++

The EC50 at 24 hours was determined to be 586 mg/l.

Test substance

: ADAMMC (80% solution in water).

Conclusion

: Under the conditions of this test, the test substance has to be regarded as slightly toxic to bacteria.

Reliability

: (1) valid without restrictions.
Guideline study.

06.11.2003

(8)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4. Ecotoxicity

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4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	: LD50
Reference	: Clouzeau, J. (1990).
Units	: mg/kg bw
Value	: 1,600 < LD50 < 2,000.
Species	: Rat.
Strain	: Sprague-Dawley.
Sex	: Male & female.
Number of animals	: 5 male at all dose levels, and 5 female at 3 dose levels.
Body weight	: Males: 188 ± 8 g; females: 144 ± 5 g.
Vehicle	: Methylcellulose.
Doses	: 500 – 2,900 mg/kg.
Observation	: 15 days.
Method	: OECD Guidelines for the Testing of Chemicals, Number 401, February, 1987: "Acute Oral Toxicity".
Year	: 1990.
GLP	: GLP.
Remark	: LD50 calculated on the basis of pure active substance.
Test procedure	: In a pilot study, the test substance was administered orally as is at a dose of 500 mg/kg body weight taking into account a specific gravity of d=1.12. Since the mortality in this study was 40%, a second test was conducted at doses of 500, 900, 1,600, 2,000 and 2,900 mg/kg for the males and 900, 1,600 and 2,000 mg/kg for the females. The test substance was administered in solution in 0.5% methylcellulose at a dose of 10 ml/kg. The animals were observed frequently during the immediate post-administration period and clinical signs were recorded.
Result	: Animals showed sedation, ataxia, abdominal/side position and reduced food uptake. Dyspnia was observed in 1 male at the 1,600 mg/kg group and in most of the animals for a period of 1 hour in the 2,900 mg/kg group. 15 minutes following administration, a red-colored eye secretion was observed over 15 minutes in 2 males in the 1,600 mg/kg group, 2 males and 1 female in the 2,000 mg/kg group and 4 males in the 2,900 mg/kg group. Cumulative mortality, in males, females and combined is given in the following table:

Sex	Dose mg/kg	Cumulative Mortality				Mortality %
		Day 1	Day 2	Day 5	Day 15	
Males	500	0	0	0	0	0
	900	0	0	0	0	0
	1,600	0	2	2	2	40
	2,000	5	5	5	5	100
	2,900	3	5	5	5	100
Females	900	0	1	1	1	20
	1,600	0	0	0	0	0
	2,000	5	5	5	5	100

The LD50 was determined to be between 1,600 and 2,000 mg/kg body

5. Toxicity

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	weight.
Test substance	: ADAMMC (80% solution in water)
Conclusion	: Under the conditions of this test, the LD50 of the test substance by the oral route in male rats is between 1,600 (40% mortality) and 2,000 mg/kg (100% mortality) body weight. The LD50 for females is slightly higher. The test substance is therefore regarded as being of low toxic concern.
Reliability	: (1) valid without restrictions. Guideline study.
05.11.2003	(9)
Type	: LD50
Reference	: Collier, T. A. (1985a).
Units	: mg/kg bw
Value	: 200 < LD50 < 2,000
Species	: Rat.
Strain	: Sprague-Dawley.
Sex	: Male & female.
Number of animals	: 4 per dose (2 male and 2 female) in the rangefinding study and 10 per dose (5 male and 5 female) in the main study.
Body weight	: Males: 101 – 111 g, females: 94 – 112g.
Vehicle	: Water.
Doses	: 25 – 5,000 mg/kg bw.
Observation	: 14 days.
Method	: OECD Guidelines for the Testing of Chemicals, Number 401, February, 1987: "Acute Oral Toxicity".
Year	: 1985
GLP	: Yes
Remark	: LD50 calculated on the basis of pure active substance.
Test procedure	: A pilot study, was carried out at 4 pre-specified dose levels (25, 200, 2,000 and 5,000 mg/kg body weight) using groups of 4 rats (2 male and 2 female) in order to determine the highest of these level that produced no mortality. All rats were dosed once only by gavage using a metal cannula attached to a graduated syringe. The dose volume administered to each animal was calculated according to its body weight at the time of dosing. Animals were observed at 0.5, 1 and 4 hours following then once daily for 5 days, or until signs of toxicity were no longer apparent. Mortality and evidence of overt toxicity were recoded at each observation. A group of 10 rats (5 male and 5 female) were dosed once at 200 mg/kg body weight (the highest dose level in the pilot study that caused no mortality).

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Result

- : An abnormal body carriage (hunched posture), lethargy, pilo-erection and decreased respiratory rate were observed in rats at 25, 200 and 2,000 mg/kg. In addition, body tremors, ataxia, increased salivation and dried blood around the eyes were seen at the 2,000 mg/kg dose level only. All animals dosed at 5,000 mg/kg died within 30 minutes of treatment. Cumulative mortality, in males, females and combined is given in the following table:

Sex	Dose mg/kg	Cumulative Mortality				Mortality %
		Day 1	Day 2	Day 5	Day 15	
Males	25	0	0	0	0	0
	200	0	0	0	0	0
	2,000	0	1	1	1	50
	5,000	2	2	2	2	100
	Second Study					
	200	0	0	0	0	0
Females	0	0	0	0	0	0
	200	0	0	0	0	0
	2,000	0	0	0	0	0
	5,000	2	2	2	2	100
	Second Study					
	200	0	0	0	0	0

The LD50 was determined to be between 200 and 2,000 mg/kg body weight.

Test substance

- : ADAMMC (80% solution in water)

Conclusion

- : Under the conditions of this test, the LD50 of the test substance by the oral route in male rats is between 200 (0% mortality) and 2,000 mg/kg (100% mortality) body weight. The test substance is therefore regarded as being of low toxic concern.

Reliability

- : (1) valid without restrictions.
Guideline study.

05.11.2003

(10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species

- : Rabbit.

Reference

Collier, T. A. (1985b).

5. Toxicity

Id 44992-01-0

Date 05.11.2003

Strain : New Zealand white.
Concentration : 80 % active substance.
Exposure : Intact and abraded skin, occlusive.
Exposure time : 4 hours.
Number of animals : 3
Body weight : 2.28 – 2.44 kg.
Observation : 24, 48 and 72 hours.
Vehicle : None.
Result : Not irritating.
Method : OECD Guidelines for the Testing of Chemicals, Number 404, February, 1987: "Acute Dermal Irritation/Corrosion".
Year : 1985
GLP : Yes.
Test procedure :

Approximately 24 hours prior to the commencement of the test, each of a group of 3 rabbits by closely clipping the fur from the dorsal/flank areas. Only animals with a healthy epidermis were selected for the study.

On the day of the test, a suitable test site was selected on the back of each rabbit. A quantity of 0.5 ml of the test material was introduced under a semi-occlusive patch which consisted of a 2.5 cm² of surgical gauze 2 layers thick. The material was held in contact with the skin by the patch which was secured in position with 2 lengths of adhesive strapping. In addition, to prevent access to the patch, the trunk of each rabbit was wrapped in an elasticated corset. The material was kept in contact with the skin for a period of 4 hours.

At the end of the exposure period, the corset was removed from each animal and the patches carefully taken off the test sites. Any residual material was immediately removed by gentle swabbing with cotton wool soaked in water.

Patches were scored at 24, 48 and 72 hours according Draize (1959).

Result : According to the Draize evaluation scheme, a primary irritation index (intact/abraded skin) of 0.00 was determined. The following indices were obtained for the intact clipped skin:

	24 hours	48 hours	72 hours	Total
Erythema	0	0	0	0
Edema	0	0	0	0

The test substance was determined to be non-irritating to rabbit skin.

Test substance : ADAMMC (80% solution in water)
Conclusion : ADAME MC was determined to be non-irritating.
Reliability : (1) valid without restrictions.
Guideline study.

07.11.2003

(11)

5.2.2 EYE IRRITATION

Species : Rabbit.
Reference : Collier, T. A. (1985c).
Strain : New Zealand white.
Concentration : 80 % active substance.
Exposure : Eye.
Exposure time : Test substance was administered in a single application.
Number of animals : 1

5. Toxicity

Id 44992-01-0

Date 05.11.2003

Body weight : 2.85 kg
Observation : 1 and 24 hours.
Vehicle : None.
Result : Moderately irritating.
Method : OECD Guidelines for the Testing of Chemicals, Number 405, February, 1987: "Acute Eye Irritation/Corrosion".
Year : 1985.
GLP : Yes.
Test procedure : A volume of 0.1 ml of the test material was instilled in the right eye of the rabbit by gently pulling the lower lid away from the eyeball to form a cup into which the test material was dropped. The upper and the lower eyelids were held together for about 1 second immediately after application to prevent loss of test material. Assessment of damage/irritation was made 1 hour and 24 hours following treatment according to the numerical scheme of Draize (1959). Examination of the eye was facilitated by use of a standard ophthalmoscope.

Result : A dulling of the normal luster of the cornea was observed at the 1-hour reading and by the 24-hour reading diffuse corneal opacity was observed. A diffuse beefy red coloration of the conjunctivae accompanied by severe swelling and extensive discharge was observed at the 1-hour reading. Similar reactions persisted at the 24-hour reading and were accompanied by areas of hemorrhage and necrosis over the conjunctivae and nictitating membranes. the results from the scoring according to the Draize method are given in the following table:

	1 hours	24 hours
Cornea		
E. Degree of Opacity	Dulling	1
F. Area of Opacity	4	1
Score (ExF) x 5	0	5
Iris (D)	1	1
Score (Dx5)	5	5
Conjunctivae		
A. Redness	3	3
B. Chemosis	4	4
C. Discharge	3	3
Score (A+B+C) x 2	20	20
Total Score	25	30

The test substance was determined to be moderately irritating to eyes.

Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC was determined to be moderately irritating to eyes.
Reliability : (1) valid without restrictions.
Comparable to guideline study.

05.11.2003

(12)

5.3 SENSITIZATION

5. Toxicity

Id 44992-01-0

Date 05.11.2003

- Species** : Guinea pig.
Reference : Collier, T.A. (1985d).
Concentration : Intradermal induction: 0.1% in water, intra-cutaneous.
Topical induction: 25% active substance, intra-cutaneous.
Challenge: undiluted, occlusive, epicutaneous.
- Number of animals** : 20
Method : OECD Guidelines for the Testing of Chemicals, Number 406 "Skin Sensitization" (Guinea Pig Maximization Test).
- Year** : 1985
GLP : Yes.
Test procedure : On Day 0, the experimental group was shaved. Into the shaved area were injected 0.1 ml of Freund's complete adjuvant, 0.1 ml of the test substance at 1% in water and 0.1 ml of a 50-50 mixture of 1% test material with Freund's adjuvant. On Day 7, the experimental group was shaved and test material at a concentration of 25% was applied to a 2 cm by 4 cm patch. Slick water-proof adhesive strapping was used to hold patch in position. the dressing was removed after 48 hours. On Day 21, the experimental group was shaved and test material applied to the clipped, right flank of each animal. Vehicle alone was applied to the left flank. Both patches were covered with an overlapping length of aluminum foil and left for 24 hours. patches were removed and the exposure site washed and marked. On Day 24, the reaction sites were scored. Appropriate solvent controls were used in this study.
- Result** : No reaction was seen in the solvent controls. The results of the scoring out of a maximum of 4 are given in the following table:

Animal number	24 hours		48 hours	
	Test	Vehicle	Test	Vehicle
1	2	0	2	0
2	1	0	1	0
3	2	0	2	0
4	1	0	1	0
5	2	0	2	0
6	2	0	2	0
7	2	0	2	0
8	2	0	1	0
9	2	0	1	0
10	2	0	2	0
11	2	0	1	0
12	2	0	1	0
13	2	0	2	0
14	1	0	1	0
15	1	0	1	0
16	2	0	2	0
17	3	0	2	0
18	2	0	2	0
19	2	0	2	0
20	Died Day 7			

The test substance was determined to be a strong sensitizer.

- Test substance** : ADAMMC (80% solution in water)
Conclusion : ADAMMC was determined to be sensitizing.
Reliability : (1) valid without restrictions
Comparable to guideline study.

06.11.2003

(13)

5. Toxicity

Id 44992-01-0

Date 05.11.2003

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Reverse Mutation Assay (Ames Test).
Reference : Clouzeau J. (1991).
System of testing : *Salmonella typhimurium* TA1535, TA1537, TA1538, TA98 and TA100
Test concentration : 10 – 5000 µg/plate
Metabolic activation : With and without.
Result : Negative.
Method : OECD Guidelines for the Testing of Chemicals, Number 471, May 1983: "Genetic Toxicology: *Salmonella Typhimurium* Reverse Mutation Assay"
Year : 1991
GLP : Yes.
Method : The test compound was evaluated in triplicate cultures in strains TA1535, TA1537, TA1538, TA98 and TA100 in the presence and absence of S9 at doses of 10, 100, 1,000, 2,500 and 5,000 µg/plate.
Result : No toxicity was observed in the background lawn. The ratio of revertants in treated plates versus controls never exceeded 1.6. No significant increase in mutations either in presence or absence of S-9.
Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC was not mutagenic in this *in vitro* assay.
Reliability : (1) valid without restrictions
Guideline study.

06.11.2003

(14)

Type : Cytogenetic assay.
Reference : Adams, K. (1990)
System of testing : Human lymphocytes.
Test concentration : 0 – 3,000 µg/plate
Metabolic activation : With and without.
Result : Negative.
Method : OECD Guidelines for the Testing of Chemicals, Number 473, 1983: "Genetic Toxicology: *In Vitro* Mammalian Cytogenetic Test".
Year : 1990.
GLP : Yes.
Method : Human blood was collected, washed 3 times and suspended at a concentration of 1×10^6 cells. 5ml-aliquots were incubated at 37°C for 48 hours. Test compound was added to give final concentration of 9.8, 19.5, 39.1, 78.2, 156, 313, 625, 1,250, 2,500 and 5,000 µg/ml (positive and negative controls were used). For metabolic activation 1.25 ml S9 was added to each culture. Cultures were incubated for 24 hours (2 hour exposure). Colchine was added to each culture. After 2 hours, cells were centrifuged, collected and fixed. Slides were stained using Giemsa solution. Metaphase figures were identified and chromosomes analyzed.
Result : While a small increase in chromosomal damage was seen at the highest dose this increase, 2.5% aberrant cells fell within historical control range and was not considered to be indicative of clastogenic activity. No compound-related effect was seen in the presence of metabolic activation.
Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC was not clastogenic in this *in vitro* assay.
Reliability : (1) valid without restrictions
Guideline study.

06.11.2003

(15)

5. Toxicity

Id 44992-01-0

Date 05.11.2003

Type : Mammalian cell gene mutation assay.
Reference : Wollny, H-E. (1997).
System of testing : Mouse lymphoma (TK⁺/-) L5178Y cells
Test concentration : 30 – 3,000 µg/plate
Metabolic activation : With and without.
Result : Negative.
Method : OECD Guidelines for the Testing of Chemicals, Number 476, April 4, 1984: "Genetic Toxicology: *In Vitro* Mammalian Cell Gene Mutation Test"
Year : 1997
GLP : Yes.
Method : Cells were suspended in medium with test article in the presence or absence of S9 metabolic activation for 4 hours. Article was removed by centrifugation and cells washed twice. Cells were plated to determine cell density (cloning efficiency). Cells were selected in the presence of 100 µg/ml TFT after 14 days.
Result : The highest concentration applied produced a decrease of cell culture growth and the cell growth observed at the lowest concentration was approximately in the range of the negative control. No precipitation of test article was observed. No substantial and reproducible increase in mutant colony numbers was observed at any valuated concentration neither in the presence or absence of metabolic activation. Furthermore, there was no indication of a dose-dependant increase in the number of spontaneous mutant colonies in the solvent control. In this study the range of negative controls was from 31 up to 47 mutant colonies per 10⁶ cells; the range of groups treated with test article was from 29 up to 68 mutant colonies per 10⁶ cells.
Test substance : ADAMMC (80% solution in water)
Conclusion : ADAMMC did not demonstrate mutagenic potential in this *in vitro* assay.
Reliability : (1) valid without restrictions
Guideline study.

07.11.2003

(16)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5. Toxicity

Id 44992-01-0
Date 05.11.2003

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 44992-01-0

Date 05.11.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

7. Eff. Against Target Org. and Intended Uses

Id 44992-01-0

Date 05.11.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.

Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.

05.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.

05.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.

In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.

In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower lids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.

If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.

In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.

05.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.

05.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.

05.11.2003

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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- (2) Calmels, R. (1994a). Test to evaluate acute toxicity (96 hours) in freshwater fish (*Brachydanio rerio*) using a static method – ADAM MeCl. Société d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (3) Wehrhahn, D. (1999) Acute Fish Toxicity of Adam-Quat on *Danio rerio* (Zebra Fish). Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany
- (4) Calmels, R. (1994b). Test to Evaluate Acute Toxicity(48 hours) in Daphnia – ADAM MeCl. Société d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (5) Wehrhahn, D. (1999b) Acute Daphnia Toxicity of Adame-Quat on *Daphnia magna*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany
- (6) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae - ADAM MECL. Société d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (7) Wehrhahn, D. (1999c) Chronic Alga Toxicity of Adame-Quat on *Scenedesmus subspicatus*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany
- (8) Wehrhahn, D. (1999d) Chronic Bacteria Toxicity of Adame-Quat on *Pseudomonas putida*. Stockhausen GmbH and Co. KG, Laboratory for Toxicology and Ecology, Krefeld, Germany
- (9) Clouzeau, J. (1990). ADQUAT MC 80 Evaluation de la toxicité aiguë par voie orale chez le rat. Centre International de Toxicologie (CIT), Miserey, France
- (10) Collier, T.A. (1985a). Range Finding Oral Toxicity Test: An Assessment of the Acute Oral Toxicity of ADQUAT 80 MC in the Rat, Safepharm Laboratories, Derby, UK.
- (11) Collier, T.A. (1985b). OECD Skin Irritation Test: Determination of the Degree of Primary Cutaneous Irritation Caused by ADQUAT 80 MC in the Rabbit. Safepharm Laboratories, Derby, UK.
- (12) Collier, T.A. (1985c). OECD Eye Irritation Test: Determination of the Degree of Ocular Irritation Caused by ADQUAT 80 MC in the Rabbit. Safepharm Laboratories, Derby, UK.
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- (14) Clouzeau, J. (1991). Acryloxyethyltrimethylammonium Chloride (80% Solution in Water) (ADAMQUAT MC 80) - Reverse Mutation Assay by the Ames Test. Centre International de Toxicologie (CIT), Miserey, France,
- (15) Adams, K. (1990). ADAMQUAT MC 80: Metaphase Chromosome Analysis of Human Lymphocytes Cultured *In Vitro*. Huntington Laboratories, Cambridgeshire, UK.
- (16) Wollny, H-E. (1997). Cell Mutation Assay at the Thymidine Kinase (TK^{+/+}) Locus in Mouse Lymphoma L5178Y Cells with DMAEA.MCQ Monomer. RCC, Rossdorf, Germany.

10. Summary and Evaluation

Id 44992-01-0

Date 05.11.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15210 B2

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I U C L I D

Data Set

Existing Chemical : Substance ID: 13106-44-0
CAS No. : 13106-44-0
TSCA Name : Ethanaminium, *N,N,N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, methyl sulfate
Structural formula : CH2=CHCOOC2H4N(CH3)3.CH3SO4
Molecular formula : C7H16NO6S
Molecular weight : 269.32

Producer related part
Company : Quat HPV Challenge Task Group
Creation date : 03.11.2003

Substance related part
Company : Quat HPV Challenge Task Group
Creation date : 03.11.2003

Number of pages : 22

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4

1. General Information

Id 13106-44-0

Date 03.11.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	: Organic.
Physical status	: Solid.
Purity	: > 99%.
Remark	: The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

03.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylacrylate, dimethyl sulfate
03.11.2003

Dimethylaminoethyl acrylate methyl sulfate
03.11.2003

[2-(acryloyloxy)ethyl]trimethylammonium methyl sulfate
03.11.2003

[(Acryloyloxy)ethyl]trimethylammonium methyl sulfate
03.11.2003

ADAM DMS
03.11.2003

DMAEA DMS
03.11.2003

1.3 IMPURITIES

1. General Information

Id 13106-44-0
Date 03.11.2003

Dimethylaminoethylacrylate (<0.1%).
04.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
04.11.2003

1.6.2 CLASSIFICATION

Not Regulated
04.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type : Industrial
Category : Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark : Commercial product is manufactured and shipped as a solution in water (75–80%).
04.11.2003

1.7.1 DETAILED USE PATTERN

Type : Industrial.
Category : Chemical industry; used in synthesis.
Remark : Water-soluble polymers. Flocculants. Retention aids.
04.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of dimethyl sulfate with dimethylaminoethylacrylate.
04.11.2003

1.8 REGULATORY MEASURES

None

1. General Information

Id 13106-44-0

Date 03.11.2003

04.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None

04.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethacrylate (ADAM) at less than 0.1%.

04.11.2003

1.8.3 WATER POLLUTION

Not applicable

04.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable

04.11.2003

1.8.5 AIR POLLUTION

Not applicable

04.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).

04.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable

04.11.2003

1.9.2 COMPONENTS

Pure substance (in aqueous solution).

04.11.2003

1.10 SOURCE OF EXPOSURE

1. General Information

Id 13106-44-0

Date 03.11.2003

None
04.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

2. Physico-Chemical Data

Id 13106-44-0

Date 03.11.2003

2.1 MELTING POINT

Value : =211.70°C.
Method : MPBPWIN v1.40.
Year : 2003.
GLP : No.
Test substance : ADAMDMS (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

2.2 BOILING POINT

Value : =498.07°C
Method : MPBPWIN v1.40 (adapted Stein & Brown method).
Year : 2003.
GLP : No.
Test substance : ADAMDMS (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

2.3 DENSITY

Type : Density
Value : = 1.12 g/cm3 at 20°C
Method : other: no data
Year : no data
GLP : no data
Test substance : ADAMDMS(80% solution in water)
Reliability : (4) not assignable
Only short information available (safety data sheet)

05.11.2003

2.3.1 GRANULOMETRY

Not applicable.
05.11.2003

2.4 VAPOUR PRESSURE

Value : =3.18 E-10 mm Hg at 25°C
Method : MPBPWIN v1.40 (modified Grain method).
Year : 2003.
GLP : No.
Test substance : ADAMDMS (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

2. Physico-Chemical Data

Id 13106-44-0

Date 03.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : Octanol-water.
log Pow : = -1.40
Method : KOWWIN v1.66.
Year : 2003
GLP : No.
Test substance : ADAMDMS (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water.
Value : Completely miscible.
Method : Other: no data.
GLP : No data.
Test substance : ADAMDMS (pure substance)
Reliability : (4) not assignable.
Only short information available (safety data sheet).

05.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value : 30-50 mPa.s
Method : Other: no data.

2. Physico-Chemical Data

Id 13106-44-0

Date 03.11.2003

GLP : No data.
Test substance : ADAMDMS (80%).
Reliability : (4) not assignable.
Only short information available (safety data sheet).

04.11.2003

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 13106-44-0

Date 03.11.2003

3.1.1 PHOTODEGRADATION

Type : Air.
Method : AOPWIN v1.90.
Year : 2003.
GLP : No.
Result : The atmospheric degradation behavior was assessed using AOPWIN (v. 1.90). An overall OH rate constant of $25.6167 \text{ E-12 cm}^3/\text{molecule}\cdot\text{sec}$ was obtained. The following half-lives can be predicted under the chosen conditions:
0.418 days (12h-day, $1.5 \text{ E6 OH}/\text{cm}^3$); 5.010 hours.
Overall ozone rate constant = $0.175 \text{ E-17 cm}^3/\text{molecule}\cdot\text{sec}$.
Half-life = 6.549 days (at $7 \text{ E11 mol}/\text{cm}^3$)
Test substance : ADAMDMS (pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

3.1.2 STABILITY IN WATER

Type : Abiotic (hydrolysis).
Method : HYDROWIN v1.67
Year : 2003.
GLP : No.
Remark : The estimated hydrolysis half-life of this substance at:
pH 7 = 9.001 years;
pH 8 = 328.762 days
Test substance : ADAMDMS (pure substance)
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : Volatility.
Media : Water – air.
Method : HENRYWIN v3.10.
Year : 2003.
Remark : The value obtained for for Henry's constant was calculated as:
Bond contribution method: $7.01 \text{ E-19 atm}\cdot\text{m}^3/\text{mole}$ (group contribution calculation incomplete). According to Thomas (1990), the substance may be considered as "not volatile from water".

3. Environmental Fate and Pathways

Id 13106-44-0

Date 03.11.2003

Test substance : Henry's LC (VP/WSol estimate using EPI values) = 1.353 E-13 atm-m³/mole
Reliability : ADAMDMS (pure substance).
: (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

05.11.2003

Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	5.01 E-10	9.42	1000
Water	49.8	900	1000
Soil	50.1	900	1000
Sediment	0.0918	3.6 E3	0

Persistence time = 789 hours.

Conclusion : Regardless of the media to which ADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of ADAMMC will be 50.1% in soil, 49.8% in water, <0.1% in sediment, and virtually nothing in air.

Test substance : ADAMDMS (pure substance)
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

3.3.2 DISTRIBUTION

Media : air – biota – sediment(s) – soil – water
Method : calculation according to Mackay, Level 1
Year : no data
Remark : The following parameters were employed in this calculation:
vapor pressure: 1.8 E-5 Pa (20°C) (calculated)
molecular weight: 207.7 g/mol
water solubility: ca. 6000 g/l (20°C) (calculated)
logPow: -2.55 (25°C) (calculated)
Result : The following environmental distribution was predicted:
water: ca. 100%, other environmental compartments below 0.001%
Reliability : (2) valid with restrictions
Generally accepted method of calculation with restrictions

04.11.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3. Environmental Fate and Pathways

Id 13106-44-0
Date 03.11.2003

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static.
Species : *Brachydanio rerio* (Zebra fish) (Fish, fresh water).
Reference : Calmels, R. (1994a).
Exposure period : 96 hours
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
Year : 1994
GLP : No.
Test substance : ADAMEDMS
Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.

Results :

Test Concentration (mg/L)	Mortality		
	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMDMS (80% solution in water)
Conclusion : ADAMDMS (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
 Guideline study.

03.11.2003

(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static.
Reference : Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hours.
Unit : mg/l
EC0 (immobilization) : > 100
EC50 (immobilization) : Not observed.
EC100 (immobilization) : Not observed.
Analytical monitoring : No.

4. Ecotoxicity

Id 13106-44-0

Date 03.11.2003

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "Daphnia sp., Acute Immobilization Test".
Year : 1994
GLP : No.
Test substance : ADAME DMS
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.

Results :

Concentration (mg/L)	No. of daphnia	Immobilization		
		No. after 24 hours	No. after 48 hours	% after 48 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : ADAMDMS (80% solution in water)
Conclusion : ADAMDMS (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

03.11.2003

(2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static.
Reference : Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water)
Exposure period : 72 hours
Unit : mg/l
EC_A50 (I) : 1<EC_A<10
EC_h50 (I) : >100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No.
Test substance : ADAME DMS
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

4. Ecotoxicity

Id 13106-44-0

Date 03.11.2003

Results

:

Concentration (mg/L)	Algal Concentration				% growth inhibition
	Start	24 hours	48 hours	72 hours	
0	10,000	103,472	725,000	2,867,361	0
1	10,000	61,111	487,509	2,547,222	2
10	10,000	29,267	50,000	256,944	43
100	10,000	20,833	18,056	20,833	87

The test was terminated after the range-finding phase.

Test substance

: ADAMDMS (80% solution in water).

Conclusion

: ADAMDMS (80% solution in water) significantly inhibits algal growth at concentrations greater than 10 mg/l.

Reliability

: (1) valid without restrictions
Guideline study.

03.11.2003

(3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5. Toxicity

Id 13106-44-0
Date 03.11.2003

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 13106-44-0
Date 03.11.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.

Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.

04.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.

04.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.

In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.

In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower lids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.

If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.

In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.

04.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.

04.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.

04.11.2003

8.6 SIDE-EFFECTS DETECTION**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

9. References

Id 13106-44-0

Date 03.11.2003

- (1) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio*) Using a static Method ADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (2) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia ADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (3) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae ADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.

10. Summary and Evaluation

Id 13106-44-0

Date 03.11.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15210B3

I U C L I D

Data Set

RECEIVED
OPPT CRIC
04 APR 30 PM 12:12

Existing Chemical : Substance ID: 5039-78-1
CAS No. : 5039-78-1
TSCA Name : Dimethylaminoethylmethacrylate, methyl chloride
Structural formula : $\text{CH}_2=\text{C}(\text{CH}_3)\text{COOC}_2\text{H}_4\text{N}(\text{CH}_3)_3.\text{Cl}$
Molecular formula : $\text{C}_9\text{H}_{18}\text{NO}_2.\text{Cl}$

Producer related part
Company : Quat HPV Challenge Task Group
Creation date : 12.11.2003

Substance related part
Company : Quat HPV Challenge Task Group
Creation date : 12.11.2003

Number of pages : 23

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4

1. General Information

Id 5039-78-1

Date 12.11.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	: Organic.
Physical status	: Solid.
Purity	: > 99%.
Remark	: The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

12.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Ethanaminium, *N, N, N*-trimethyl-2[(2-methyl-1-oxo-2-propenyl)oxy]-, chloride
12.11.2003

2-Trimethylammoniummethyl methacrylate chloride
12.11.2003

Choline chloride methacrylate
12.11.2003

Dimethylaminoethyl methacrylate methochloride
12.11.2003

N, N, N-Trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]ethanaminium chloride
12.11.2003

Trimethylammoniummethyl methacrylate chloride
12.11.2003

[2-(Methacryloyloxy)ethyl]trimethylammonium chloride
12.11.2003

1. General Information

Id 5039-78-1

Date 12.11.2003

[(Methacryloxy)ethyl]trimethylammonium chloride
12.11.2003

MADAM MC
12.11.2003

DMAEM MC
12.11.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type	: Industrial
Category	: Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	: Commercial product is manufactured and shipped as a solution in water (75–80%).

12.11.2003

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1. General Information

Id 5039-78-1

Date 12.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 5039-78-1

Date 12.11.2003

2.1 MELTING POINT

Value : =151.81°C.
Method : MPBPWIN v1.40.
Year : 2003.
GLP : No.
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

12.11.2003

2.2 BOILING POINT

Value : =405.99°C
Method : MPBPWIN v1.40 (adapted Stein & Brown method).
Year : 2003.
GLP : No.
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

12.11.2003

2.3 DENSITY

Type : density
Value : = 1.18 g/cm³ at 25°C (80% solution in water).
Method : other: no data
Year : no data
GLP : no data
Test substance : MADAM MC (80% solution in water)
Reliability : (4) not assignable
Only short information available (safety data sheet)

12.11.2003

(1)

2.3.1 GRANULOMETRY

Not applicable.

12.11.2003

2.4 VAPOUR PRESSURE

Value : =3.03 E-7 mm Hg at 25°C
Method : MPBPWIN v1.40 (modified Grain method).
Year : 2003.
GLP : No.
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

2. Physico-Chemical Data

Id 5039-78-1

Date 12.11.2003

12.11.2003

2.5 PARTITION COEFFICIENT

Partition coefficient : Octanol-water.
log Pow : -2.55
Method : KOWWIN v1.66.
Year : 2003
GLP : No.
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

13.11.2003

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water.
Value : Completely miscible.
Method : Other: no data.
GLP : No data.
Test substance : MADAMMC (pure substance)
Reliability : (4) not assignable.
Only short information available (safety data sheet).

13.11.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : Does not flash.
Method : Other: no data.
Year : No data.
GLP : No data.
Test substance : MADAM MC (80% solution in water).
Reliability : (4) not assignable
Only short information available (safety data sheet)

13.11.2003

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

Id 5039-78-1

Date 12.11.2003

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	: 100 mPa.s
Method	: Other: no data.
GLP	: No data.
Test substance	: MADAMMC (80%).
Reliability	: (4) not assignable.

Only short information available (safety data sheet).

13.11.2003

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 5039-78-1

Date 12.11.2003

3.1.1 PHOTODEGRADATION

Type : Air.
Method : AOPWIN v1.90.
Year : 2003.
GLP : No.
Result : The atmospheric degradation behavior was assessed using AOPWIN (v.1.90). An overall OH rate constant of $34.4425 \text{ E-12 cm}^3/\text{molecule}\cdot\text{sec}$ was obtained. The following half-lives can be predicted under the chosen conditions:
0.311 days (12h-day, $1.5 \text{ E6 OH}/\text{cm}^3$); 3.727 hours.
Overall ozone rate constant = $0.175 \text{ E-17 cm}^3/\text{molecule}\cdot\text{sec}$.
Half-life = 1.007 days (at $7 \text{ E11 mol}/\text{cm}^3$)
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

13.11.2003

3.1.2 STABILITY IN WATER

Type : Abiotic (hydrolysis).
Method : HYDROWIN v1.67
Year : 2003.
GLP : No.
Remark : The estimated hydrolysis half-life of this substance at:
pH 7 = 68.343 years;
pH 8 = 6.834 years
Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

13.11.2003

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : Volatility.
Media : Water – air.
Method : HENRYWIN v3.10.
Year : 2003.
Remark : The value obtained for for Henry's constant was calculated as:
Bond contribution method: $1.09 \text{ E-14 atm}\cdot\text{m}^3/\text{mole}$ (group contribution calculation incomplete). According to Thomas (1990), the substance may

3. Environmental Fate and Pathways

Id 5039-78-1

Date 12.11.2003

Test substance : be considered as "not volatile from water".
Reliability : Henry's LC (VP/WSol estimate using EPI values) = $8.281 \text{ E-14 atm-m}^3/\text{mole}$
: MADAMMC (100% pure substance).
: (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

14.11.2003

Type : Level III Fugacity Model
Media : Water – air – soil – sediment.
Method : BCFWIN v2.14.
Year : 2003.
Result : The value obtained from the Level III Fugacity Model are as follows:

	Mass Amount (%)	Half-Life (hr)	Emissions (kg/hr)
Air	4.12 E-7	5.7	1000
Water	45.3	360	1000
Soil	54.6	360	1000
Sediment	0.0755	1.44 E3	0

Persistence time = 421 hours.

Conclusion : Regardless of the media to which MADAMMC is released, virtually all at steady state is in the soil and water phases. Using the default emissions of equal amounts to soil, air, water and sediment (1000 kg/hr for each) the Level III model predicts that the distribution of MADAMMC will be 54.6% in soil, 45.3% in water, <0.1% in sediment, and virtually nothing in air.

Test substance : MADAMMC (100% pure substance).
Reliability : (2) valid with restrictions.
Generally accepted method of calculation with restrictions.

14.11.2003

3.3.2 DISTRIBUTION

Media : air – biota – sediment(s) – soil – water
Method : calculation according to Mackay, Level 1
Year : no data
Remark : The following parameters were employed in this calculation:
vapor pressure: 1.8 E-5 Pa (20°C) (calculated)
molecular weight: 207.7 g/mol
water solubility: $\text{ca. } 6000 \text{ g/l}$ (20°C) (calculated)
logPow: -2.55 (25°C) (calculated)
Result : The following environmental distribution was predicted:
water: ca. 100%, other environmental compartments below 0.001%
Reliability : (2) valid with restrictions
Generally accepted method of calculation with restrictions

14.11.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

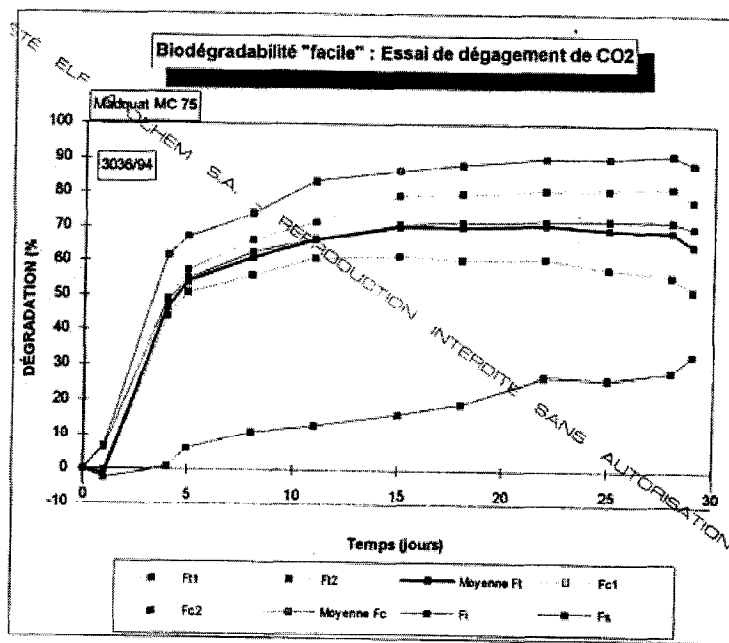
Type : Aerobic.
Reference : Thiébaud, H. (1994).

3. Environmental Fate and Pathways

Id 5039-78-1

Date 12.11.2003

Inoculum : WWTP effluent.
Concentration : 48.7 mg/l (corresponding to a DOC of 20 mg/l)
Contact time : 28 days
Degradation : = 71% after 22 days (plateau)
 = 69% after 28 days
Result : Readily biodegradable.
Deg. Product : Not measured.
Method : OECD Guidelines for the Testing of Chemicals, No. 301B, July 17, 1992: "Ready Biodegradability: Modified Sturm Test (CO₂ evolution)".
Year : 1994
GLP : Yes.
Test substance : MADAMMC (75% solution in water).
Remark : The test substance is referred to as MADQUAT MC 75
Method : Biodegradation of MADAM MC by an inoculum of 1.22×10^5 bacterium from the secondary treatment at Versailles (France) MWWTP was determined at 22°C. Percentage of CO₂ produced was determined after collection in NaOH.
Result : The maximum level of biodegradation attained was 71% after 22 days. The lag period for degradation of the test material (time from start of study until 10% degradation) was less than 5 days and the degradation 10 days after the lag period was 70%. The study met all the required validity criteria. The graphical representation of the biodegradation is shown below:



Test substance : MADAMMC (75% solution in water)
Conclusion : MADAMMC was considered to be readily biodegradable
Reliability : (1) valid without restrictions
 Guideline study.

14.11.2003

(1)

3.6 BOD5, COD OR BOD5/COD RATIO

3. Environmental Fate and Pathways

Id 5039-78-1
Date 12.11.2003

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 5039-78-1

Date 12.11.2003

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static
Reference : Calmels, R. (1994a).
Species : *Brachydanio rerio* (Zebra fish)(Fish, fresh water).
Exposure period : 96 hours.
Unit : mg/l
LC0 : > 100
LC50 : Not observed.
LC50 : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
Year : 1994.
GLP : No.
Test substance : MADAME MECL
Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.

Results

Test Concentration (mg/L)	Mortality		
	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMMC (80% solution in water)
Conclusion : MADAMMC (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003

(2)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static
Reference : Calmels, R. (1994b).
Species : *Daphnia magna* (Crustacean, fresh water)
Exposure period : 48 hours.
Unit : mg/l
EC0 (immobilization) : > 100.
EC50 (immobilization) : Not observed.
EC100 (immobilization) : Not observed.
Analytical monitoring : No.

4. Ecotoxicity

Id 5039-78-1

Date 12.11.2003

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "Daphnia sp., Acute Immobilization Test".
Year : 1994.
GLP : No
Test substance : MADAME MECL
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.

Results :

Concentration (mg/L)	No. of daphnia	Immobilization		
		No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	1	5
1	20	0	1	5
10	20	0	0	0
100	20	0	0	0

Since the EC50 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMMC (80% solution in water)
Conclusion : MADAMMC (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003

(3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static
Reference : Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water).
Exposure period : 72 hours.
Unit : mg/l
EC_A50 (I) : Not observed.
EC_P50 (I) : Not observed.
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No
Test substance : MADAME MECL
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

4. Ecotoxicity

Id 5039-78-1

Date 12.11.2003

Results

Concentration (mg/L)	Algal Concentration				% growth inhibition
	Start	24 hours	48 hours	72 hours	
0	10,000	25,965	165,972	820,833	0
1	10,000	50,000	126,399	899,611	-4
10	10,000	50,000	159,722	754,167	2
100	10,000	62,500	95,834	584,722	26

Since both the EC_{A50} and the $EC_{\mu 50}$ at 24, 48 and 72 hours were greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance

: MADAMMC (80% solution in water)

Conclusion

: MADAMMC (80% solution in water) does not significantly inhibit algal growth at 100 mg/l.

Reliability

: (1) valid without restrictions
Guideline study.

13.11.2003

(4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Ames test.
Reference	: Molinier, B. (1992).
System of testing	: <i>Salmonella typhimurium</i> TA1535, TA1537, TA1538, TA98 and TA100
Test concentration	: 312.5 – 5000 ug/plate
Metabolic activation	: With and without S9.
Result	: Negative
Method	: OECD Guidelines for the Testing of Chemicals, No. 471 "Genetic Toxicology: <i>Salmonella typhimurium</i> Reverse Mutation Assay".
Year	: 1992
GLP	: Yes.
Test substance	: MADAMMC (75% solution in water)
Method	The test compound was evaluated in triplicate cultures in strains TA1535, TA1537, TA1538, TA98 and TA100 in the presence and absence of S9 at the above doses. (Ames <i>et al</i> , 1975)
Result	The ratio of revertants in treated plates versus controls never exceeded 1.4. No significant increase in mutations either in presence or absence of S-9.
Test substance	: MADAMMC (75% solution in water)
Conclusion	: MADAMMC was not mutagenic in this in vitro assay.
Reliability	: (1) valid without restrictions
	Guideline study.

13.11.2003

(5)

5. Toxicity

Id 5039-78-1

Date 12.11.2003

Type : Cytogenetic assay
Reference : Molinier, B. (1995).
System of testing : Human lymphocytes
Test concentration : 625, 1250, 2,500 and 5,000 µg/ml.
Metabolic activation : With and without.
Result : Negative.
Method : OECD Guidelines for the Testing of Chemicals, No. 473: "*In Vitro* Mammalian Chromosome Aberration Test".
Method : Human blood was collected, washed 3 times and suspended at a concentration of 1×10^6 cells. 5ml-aliquots were incubated at 37°C for 48 hours. Test compound was added to give final concentration of 625, 1250, 2,500 and 5,000 µg/ml (positive and negative controls were used). For metabolic activation 1.25 ml S9 was added to each culture. Cultures were incubated for 24 hours (2 hour exposure). Colchicine was added to each culture. After 2 hours, cells were centrifuged, collected and fixed. Slides were stained using Giemsa solution. Metaphase figures were identified and chromosomes analyzed.
Result : No significant increase in chromosomal damage was seen at any dose tested. No compound-related effect was seen in the presence of metabolic activation.
Year : 1995.
GLP : Yes.
Test substance : MADAMMC (75% solution in water)
Conclusion : MADAMMC was not clastogenic in this in vitro assay.
Reliability : (1) valid without restrictions
Guideline study.

13.11.2003

(6)

Type : Mammalian cell gene mutation assay
Reference : Adams, K. (1997).
System of testing : Mouse lymphoma (T/K⁺) L5178Y cells
Test concentration : 300 – 5000 ug/plate
Method : OECD Guidelines for the Testing of Chemicals, No. 476 "*Genetic Toxicology: In vitro* Mammalian Cell Gene Mutation Test".
Metabolic activation : With and without (S9).
Result : Negative.
Year : 1997
GLP : Yes.
Method : Cells were suspended in medium with test article in the presence or absence of S9 metabolic activation for 4 hours. Article was removed by centrifugation and cells washed twice. Cells were plated to determine cell density (cloning efficiency). Cells were selected in the presence of 100 µg/ml TFT after 14 days.
Result : The highest concentration applied produced a decrease of cell culture growth and the cell growth observed at the lowest concentration was approximately in the range of the negative control. No precipitation of test article was observed. No substantial and reproducible increase in mutant colony numbers was observed at any valuated concentration neither in the presence or absence of metabolic activation. Furthermore, there was no indication of a dose-dependant increase in the number of spontaneous mutant colonies in the solvent control. The material did not significantly increase the mutant frequency in this test.
Test substance : MADAMMC (75% solution in water)
Conclusion : MADAM MC did not demonstrate mutagenic potential in this *in vitro* assay.
Reliability : (1) valid without restrictions
Guideline study.

5. Toxicity

Id 5039-78-1

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(7)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 5039-78-1

Date 12.11.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS OF HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product. When using, do not smoke. Handle in accordance with good industrial hygiene and safety practice.

Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.

14.11.2003

8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.

14.11.2003

8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.

In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.

In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower lids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.

If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.

In case of accidental release, do not allow product to enter drains. Do not contaminate water. Dam up spills. Soak with inert absorbent material. If liquid has been spilled in large quantities, clean up promptly by scoop or vacuum. Keep in suitable and closed containers for disposal. After cleaning, flush area with water.

14.11.2003

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.

14.11.2003

8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.

14.11.2003

8.6 SIDE-EFFECTS DETECTION**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

- (1) Thiébaud, H. (1994). MADQUAT MC 75 - Détermination de la Biodégradabilité Facile. Essai de Dégagement de CO₂. Elf-Atochem, Centre d'Application de Levallois-Perret, Levallois, France.
- (2) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio*) Using a static Method MADAM MECL. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (3) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia MADAM MECL. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (4) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae MADAM MECL. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (5) Molinier B. (1992). MADQUAT MC 75: Reverse Mutation Assay by the Ames test. Test Report of Elf Atochem S.A. (France).
- (6) Molinier B. (1995). MADQUAT MC 75: *In Vitro* Mammalian Cytogenic Test in Cultured Human Lymphocytes. Test Report of Elf Atochem S.A. (France).
- (7) Adams, K. (1997). MADAM-MC Mammalian Cell Mutation Assay. Huntington Laboratories, Cambridgeshire, UK.

10. Summary and Evaluation

Id 5039-78-1
Date 12.11.2003

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT

201-15210B4

I U C L I D

Data Set

RECEIVED
09 PT 0910
04 APR 30 PM 12:12

Existing Chemical : Substance ID: 6891-44-7
CAS No. : 6891-44-7
TSCA Name : Ethanaminium, N,N,N-trimethyl-2-[(2-methyl-1-oxo-2-propenyl)oxy]-, methyl sulfate
Structural formula : CH3C2H2COOC2H4N.(CH3)3.OSO3CH3
Molecular formula : C9H18NO2.CH3O4S

Producer related part
Company : Quat HPV Challenge Task Group
Creation date : 10.11.2003

Substance related part
Company : Quat HPV Challenge Task Group
Creation date : 10.11.2003

Number of pages : 18

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4

1. General Information

Id 6891-44-7

Date 10.11.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Substance type	: Organic.
Physical status	: Solid.
Purity	: > 99%.
Remark	: The commercial product is manufactured and shipped as a solution (75 – 80%) in water.

10.11.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Dimethylaminoethylmethacrylate, dimethyl sulfate
10.11.2003

Choline, methylsulfate, acrylate
10.11.2003

Ethanaminium, *N,N,N*-trimethyl-2-[(1-oxo-2-propenyl)oxy]-, methyl sulfate
10.11.2003

[2-(Acryloyloxy)ethyl]trimethylammonium methyl sulphate
10.11.2003

N,N,N-Trimethyl-2-[(1-oxo-2-propenyl)oxy]ethanaminium methyl sulfate
10.11.2003

N,N,N-Trimethyl-2-(1-oxo-2-propenyloxy)ethanaminium methyl sulfate
10.11.2003

Trimethylammonioethyl acrylate, methylsulfate salt
10.11.2003

1. General Information

Id 6891-44-7

Date 10.11.2003

(2-Acryloyloxyethyl)-N,N,N-trimethylammonium methosulfate
10.11.2003

MADAMDMS
10.11.2003

DMAEMDMS
10.11.2003

Flocryl MADAMQUAT DMS
10.11.2003

1.3 IMPURITIES

Dimethylaminoethylmethacrylate (<0.1%).
10.11.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Sensitizing. Irritating to eyes.
10.11.2003

1.6.2 CLASSIFICATION

Not Regulated
10.11.2003

1.6.3 PACKAGING

1.7 USE PATTERN

Type	: Industrial
Category	: Chemical industry; used in synthesis of water soluble polymers, flocculants, retention aids.
Remark	: Commercial product is manufactured and shipped as a solution in water (75–80%).

10.11.2003

1.7.1 DETAILED USE PATTERN

1. General Information

Id 6891-44-7

Date 10.11.2003

Used in closed system to manufacture polymers. Polymers are water-soluble and cationic and are either copolymers with acrylamide and other monomers or homopolymers.
10.11.2003

1.7.2 METHODS OF MANUFACTURE

Manufactured by reaction of dimethyl sulfate with dimethylaminoethylmethacrylate.
10.11.2003

1.8 REGULATORY MEASURES

None
10.11.2003

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

None.
10.11.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

Dimethylaminoethylmethacrylate (MADAM) at less than 0.1%.
10.11.2003

1.8.3 WATER POLLUTION

Not applicable.
10.11.2003

1.8.4 MAJOR ACCIDENT HAZARDS

Not applicable.
10.11.2003

1.8.5 AIR POLLUTION

Not applicable.
10.11.2003

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

Listed on all major chemical inventories (TSCA, EINECS, ECL, AICS, etc.).
10.11.2003

1. General Information

Id 6891-44-7

Date 10.11.2003

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

Not applicable.
10.11.2003

1.9.2 COMPONENTS

Pure substance (in aqueous solution).
10.11.2003

1.10 SOURCE OF EXPOSURE

None.
10.11.2003

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 6891-44-7

Date 10.11.2003

2.1 MELTING POINT

2.2 BOILING POINT

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

2.5 PARTITION COEFFICIENT

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2. Physico-Chemical Data

Id 6891-44-7

Date 10.11.2003

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 6891-44-7

Date 10.11.2003

3.1.1 PHOTODEGRADATION

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : Static.
 Species : *Brachydanio rerio* (Zebra fish) (Fish, fresh water).
 Reference : Calmels, R. (1994a).
 Exposure period : 96 hours
 Unit : mg/l
 LC0 : > 100
 LC50 : Not observed.
 LC50 : Not observed.
 Analytical monitoring : No.
 Method : OECD Guidelines for the Testing of Chemicals, No. 203, 1984: "Fish, Acute Toxicity Test".
 Year : 1994
 GLP : No.
 Test substance : MADAME DMS
 Test procedure : Groups of 10 fresh water Zebra fish (*Brachydanio rerio*) were exposed in a reconstituted medium at 23° C for 96 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Fish mortality was measured after 24, 48 and 96 hours.

Results :

Test Concentration (mg/L)	Mortality		
	24 hours	48 hours	96 hours
0	0	0	0
1	0	0	0
10	0	0	0
100	0	0	0

Since the LC0 at 24, 48 and 96 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAM DMS (80% in solution in water)
 Conclusion : MADAMDMS (80% solution in water) is not toxic to freshwater fish at a concentration of 100 mg/l.
 Reliability : (1) valid without restriction
 Guideline study

10.11.2003

(1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : Static.
 Reference : Calmels, R. (1994b).
 Species : *Daphnia magna* (Crustacean, fresh water)
 Exposure period : 48 hours.
 Unit : mg/l
 EC0 (immobilization) : > 100
 EC50 (immobilization) : Not observed.
 EC100 (immobilization) : Not observed.
 Analytical monitoring : No.

4. Ecotoxicity

Id 6891-44-7

Date 10.11.2003

Method : OECD Guidelines for the Testing of Chemicals, No. 202, April 1984: "*Daphnia* sp., Acute Immobilization Test".
Year : 1994
GLP : No.
Test substance : MADAME DMS
Test procedure : Groups of 10 fresh water daphnia (*Daphnia magna*) were exposed in a reconstituted medium at 23° C for 48 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Immobilized daphnia were counted after 24 and 48 hours.

Results :

Concentration (mg/L)	No. of daphnia	Immobilization		
		No. after 24 hours	No. after 48 hours	% after 24 hours
0	20	0	0	0
1	20	0	0	0
10	20	0	0	0
100	20	0	0	0

Since the EC0 at 24 and 48 hours was greater than 100 mg/L, the test was terminated after the range-finding phase.

Test substance : MADAMDMS (80% in solution in water)
Conclusion : MADAMDMS (80% solution in water) has no effect on the swimming behavior of daphnia at a concentration of 100 mg/l.
Reliability : (1) valid without restrictions
Guideline study.

10.11.2003

(2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Type : Static.
Reference : Licata-Messana, L. (1994).
Species : *Scenedesmus subspicatus* (Algae, unicellular, fresh water)
Exposure period : 72 hours
Unit : mg/l
EC_A50 (I) : 10<EC_A<100
EC_u50 (I) : >100
Analytical monitoring : No.
Method : OECD Guidelines for the Testing of Chemicals, No. 201, June 1984: "Alga, Growth Inhibition Test".
Year : 1994
GLP : No.
Test substance : MADAME DMS
Test procedure : Blue-green algae (*Scenedesmus subspicatus*) were exposed in a reconstituted medium at 23° C for 72 hours. The pH was carefully monitored throughout the study. Concentrations of 0.0, 1.0, 10, and 100.0 mg/l of test substance were used. Algal concentrations were measured after 24, 48 and 72 hours.

4. Ecotoxicity

Id 6891-44-7

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Results

:

Concentration (mg/L)	Algal Concentration				% growth inhibition
	Start	24 hours	48 hours	72 hours	
0	10,000	103,472	725,000	2,867,361	0
1	10,000	93,055	708,333	2,586,111	7
10	10,000	84,722	513,889	2,375,000	21
100	10,000	69,445	194,444	1,294,444	60

The test was terminated after the range-finding phase.

Test substance

: MADAMDMS (80% in solution in water)

Conclusion

: MADAMDMS (80% solution in water) moderately inhibits the growth of blue-green algae.

Reliability

: (1) valid without restriction
Guideline study

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(3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2 CORROSIVENESS AND IRRITATION

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

6. Analyt. Meth. for Detection and Identification

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5.9 SPECIFIC INVESTIGATIONS

5.10 OTHER RELEVANT INFORMATION

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

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7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

Avoid all contact with the product by ingestion, inhalation or contact with the skin, eyes and clothing. Do not breathe vapors or spray mist. Wash hands and face before breaks and immediately after handling the product.

Store in contact with air. Do not exceed storage temperature of 30°C. Protect from light.

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8.2 FIRE GUIDANCE

This product does not burn in aqueous solution. No special precautions required. In case of fire, wear a self contained breathing apparatus. Keep containers cool during fire with water spray.

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8.3 EMERGENCY MEASURES

If product is inhaled, move to fresh air.

In case of skin contact, rinse and wash contaminated clothing before re-use. Wash contaminated area immediately for at least 15 minutes. In case of persistent skin irritation, consult a physician.

In case of eye contact, rinse immediately with plenty of water for at least 15 minutes. Keep eye wide open while rinsing and lift upper and lower lids to ensure complete removal of chemical. In case of persistent eye irritation, consult a physician.

If swallowed, do not induce vomiting. Rinse mouth (never give anything by mouth to an unconscious person). Call a physician immediately.

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8.4 POSSIB. OF RENDERING SUBST. HARMLESS

Not applicable.

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8.5 WASTE MANAGEMENT

Can be land filled or incinerated when in compliance with local regulations.

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8.6 SIDE-EFFECTS DETECTION**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER****8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**

- (1) Calmels, R. (1994a). Test to Evaluate Acute Toxicity (96hours) in Freshwater Fish (*Brachydanio rerio*) Using a static Method MADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (2) Calmels, R. (1994b). Test to Evaluate Acute Toxicity (48hours) in Daphnia MADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.
- (3) Licata-Messana, L. (1994). Inhibition Test (72 hours) in Freshwater Unicellular Algae MADAME DMS. Societe d'Ecotoxicologie et de Physico-Chimie (SEPC), Sarcey, France.

10. Summary and Evaluation

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT